Towards a Next-Generation Reconnection-ALE Hydrocode

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The focus of our research is the development of a new Reconnection-Arbitrary-Lagrangian-Eulerian (ReALE)-based hydrocode for modeling solids and fluids subject to extreme conditions. The ReALE formulation that we are developing is based on a physically motivated and mathematically rigorous construction of the underlying Lagrangian method and vector/tensor reconstruction and remapping algorithms. This work brings together many new concepts that in combination with contemporary cell-centered Lagrangian methods will produce a cutting-edge ReALE capability and define a new state-of-the-art. The proposed research and the resulting algorithms will be of immediate use in Eulerian, Lagrangian, and Arbitrary Lagrangian Eulerian (ALE) codes in several DOE programs and codes.

Modeling real materials with finite strength is of particular interest in applications such as Inertial Confinement Fusion (ICF), munition-target interactions, geological impact dynamics, shock processing of powders, and formation of shaped charges. These applications constitute a specific class of problems in which the hydrodynamic pressure realized is often much greater than the strength of the material, thereby leading to large deformation of the interacting media. Traditionally, the tools that have been used to solve large deformation transient problems have been termed hydrocodes.

Over the past 20 years, there have been a plethora of significant hydrocode efforts based on Eulerian, Lagrangian, and ALE methods. In spite of their number, existing hydrocodes are known to exhibit multiple numerical, physical, and mathematical inconsistencies. For instance, despite the recent advancement with the Eulerian formulations, the Lagrangian framework has been widely preferred for many applications due to its ability to follow the material response. Furthermore, since many of the constitutive relations demand detailed knowledge of the material motion, Lagrangian formulations are considered to be the natural choice. On the other hand, Lagrangian formulation-based ALE methods require frequent surgical procedures to prevent mesh from tangling, particularly for applications with strong vortices. Additional pathologies stem from the use of low-order staggered-grid discretizations, ad hoc artificial viscosities, unconstrained mesh instabilities, and poor pressure-gradient approximations on distorted grids.

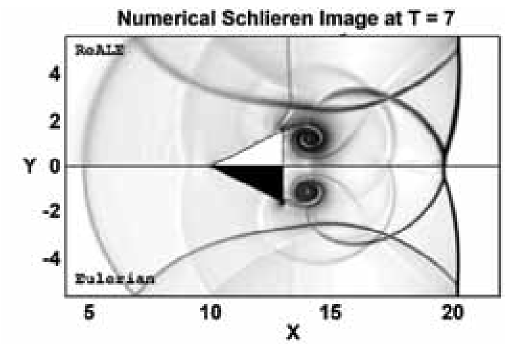

Fig. 1. Mach 1.3 shock impacting a rigid wedge.

The primary goal of this research is to develop a numerical paradigm that is devoid of the pathologies and yet faithfully represents the material behavior. In particular, we are developing a new ReALE-based hydrocode [1] for solving large deformation problems in solids and fluids. As the name indicates, ReALE permits the connectivity of the mesh to dynamically adapt to evolving features in the solution field. The reconnection part of ReALE significantly alleviates the computational encumbrance enjoined with mesh untangling procedures. Furthermore, applications with intrinsic strong vortices can be captured and treated adequately. At the heart of our algorithm lies a high-order cell-centered discretization scheme [2] that neither requires explicit artificial viscosity terms nor demands ad hoc mesh stabilization methods. The underlying construction of the scheme is generic in that advanced hypo/hyperelastic constitutive theories can be easily incorporated. Built upon this emerging cell-centered scheme are the physically motivated and mathematically consistent, frame invariant and symmetry preserving, vector/tensor reconstruction, limiting, and remapping techniques. Consequently, we are aiming to remove numerical and physical inconsistencies at a more fundamental level. Together with these significant improvements, we are establishing the next generation ReALE hydrocode as an alternative to Eulerian and ALE methods.

Our preliminary investigation demonstrates an impressive outcome for applications involving fluid and solid media subject to extreme conditions. The capability of the formulation in capturing dominant features in the solution field is evinced in Figs 1, 2, 3, and 4. In these figures, the new ReALE formulation-based solution is compared against well-established Eulerian methods [3] for problems that are inherently Eulerian in nature. In Fig. 1, we demonstrate the ability to capture strong vortical structures in the flow field. A Mach 1.3 shock impacting a wedge-shaped rigid obstruction generates a complex shock-vortical system. Comparison with Eulerian simulation indicates remarkable agreement between the two calculations. Figure 2 gives a snapshot of the shock diffraction patterns in water that are generated from the interaction of a Mach 1.4 shock wave with an air cavity. In Figs 3 and 4, the deformation of a copper rod and a hemispherical groove (in copper),

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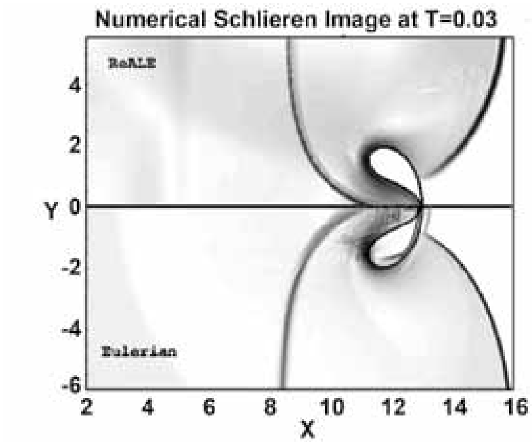

Fig. 2. Shock diffraction patterns in water.

due to high-impact conditions, are presented. The latter example is a prototype for analyzing explosively formed projectiles. Throughout these and other computations that we have investigated, the new ReALE formulation is found to be at par with existing Eulerian methods.

The development of this new paradigm, which dramatically reduces physical, numerical, and mathematical anomalies, is an important research issue that will affect multiple DOE programs and codes. This effort will provide the necessary research on algorithms for treating hypo/hyperelastic plastic materials and reconstruction and remapping of the tensor quantities required to advance new and existing hydrocodes. Specifically, the research and resulting algorithms will be of immediate use in Eulerian, Lagrangian, and ALE hydrocodes developed under the Advanced Simulation and Computing Program. In the future, we will be extending the formulation to accurately treat embedded material interfaces. Furthermore, efforts are already underway for solving 3D applications using the advanced computing facilities available at LANL.

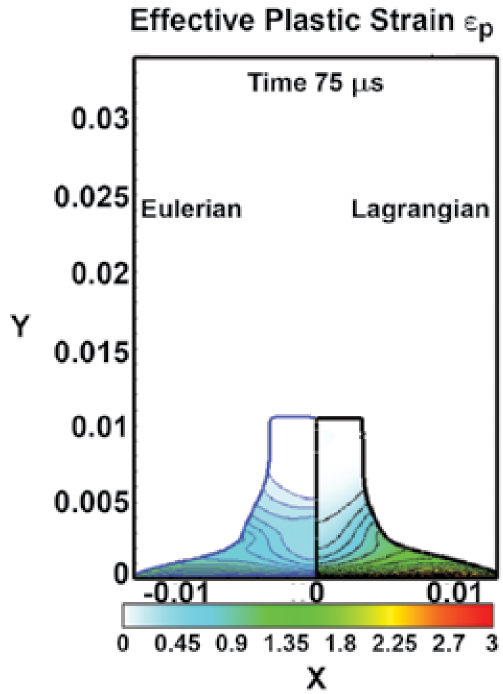

Fig. 3. Deformation of copper rod impacting rigid wall at 400 m/s.

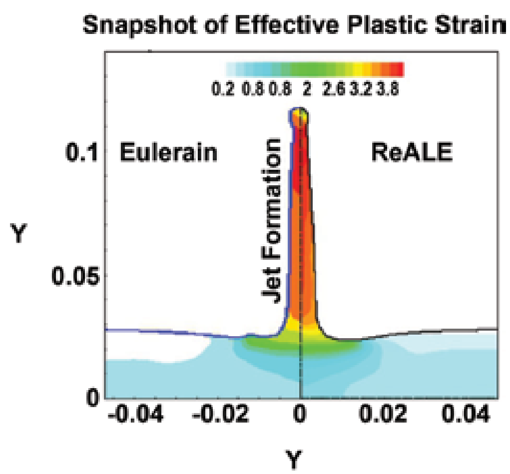

Fig. 4. Formation of jet due to the impact of shock wave on a hemispherical groove in copper.

[1] Loubere, R. et al., *J Comput Phys* **229**(12), 4724 (2010).

[2] Sambasivan, S. et al., "A Cell-Centered Lagrangian Finite Volume Approach for Computing Elasto-Plastic Response of Solids in Cylindrical Axisymmetric Geometries," LA-UR 12-20947, *J Comput Phys*, **237**, (2013).

[3] Sambasivan, S. et al., "Simulation of Collapse and Fragmentation Phenomena in a Sharp Interface Eulerian Setting," LA-UR 12-23179, *J Comput Phys*, **235,** 334 (2013).